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Electron scattering in two-dimensional disordered heterostructures

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ABSTRACT

The main aim of this work is to study electron scattering in imperfect semiconductor heterostructures. The source of unintentional disorder is the interface roughness at the heterojunctions occurring during growth. In order to achieve this goal we solve numerically the two-dimensional Ben Daniel-Duke equation for the electron scattering problem. Our model assumes open boundary conditions along the growth direction and periodic ones parallel to the heterojunctions. We then compute the reflection and transmission matrices that govern channel mixing due to interface roughness scattering. The knowledge of the mixing matrices allow us to calculate the transmission coefficient in any heterostructure made of wide gap semiconductors. As an example, we compute the transmission coefficient in resonant tunneling devices based on double-barrier structures.

INTRODUCTION

Electron scattering by imperfect heterojunctions reduces electron mobility due to rough surfaces even in good-quality heterostructures [1]. So far, there are analytical results concerning the propagation of wave packets in a randomly layered medium when the potential is a random function of only one coordinate [2], but for a small number of layers, as in double barrier heterostructures (DBH), in-plane disorder becomes important and one expects such approaches to fail. Realistic models of in-plane disorder usually lead to intractable analytical models; hence the importance of numerically solvable models to bridge this gap. An important contribution was already provided by Henrickson *et al.*, who applied the tight-binding Green function method to account for electron scattering by interface roughness in imperfect DBH [3]. However, in this paper electron transmission through a DBH was described by a rather artificial model of disorder, namely periodic roughness with random relative phases at the interfaces.

In the present work we introduce a two-dimensional effective-mass model to study the effects of interface roughness scattering on electron transmission through semiconductor heterostructures. To this end, the Ben Daniel-Duke equation is discretized, boundary conditions are discussed and scattering solutions are found by means of the transfer-matrix method for *any* arbitrary heterostructure made of wide gap semiconductors. The model is worked out in a two-dimensional space for computational limitations, although it will be clear that generalization to three dimensions is rather straightforward. Finally, we present the numerical results for the transmission coefficient through imperfect DBH and the main conclusions of the work.

THEORY

We consider the Ben Daniel-Duke equation with constant effective mass m^* at the Γ valley for the electron envelope function $\psi(y, z)$, where the two spatial directions are shown in Fig. 1. The whole structure is divided into three different regions, namely left (I) and right (III) contacts and the DBH (II), where scattering by lateral disorder takes place.

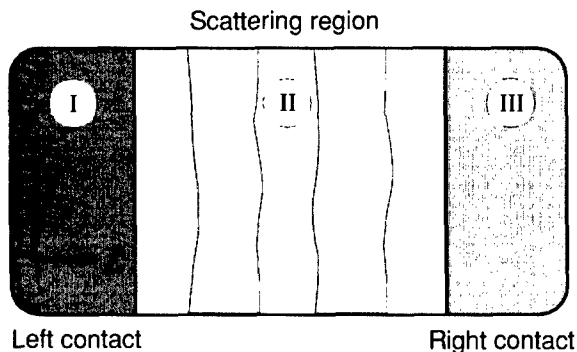


Figure 1. Schematic view of the sample. Regions I and III are the electrical contacts of the sample and electrons undergo scattering processes by lateral disorder only at region II (DBH).

We consider a mesh with lattice spacings a_y and a_z in the y and z directions, respectively. Defining $t_y \equiv -\hbar^2/(2m^*a_y^2)$ and $t_z \equiv -\hbar^2/(2m^*a_z^2)$, we obtain the discretized equation for the envelope function

$$t_z(\psi_{n+1,m} + \psi_{n-1,m}) + t_y(\psi_{n,m+1} + \psi_{n,m-1}) + (U_{n,m} - 2t_z - 2t_y)\psi_{n,m} = E\psi_{n,m}. \quad (1)$$

The potential term $U_{n,m}$ in Eq. (1) is given by the conduction-band edge energy at the point (na_y, ma_z) which, in turn, depends on the Al mole fraction in the vicinity of that position. Therefore, lateral disorder enters the equation through this diagonal term. Contacts are characterized by flat band conditions, $U(n, m) = 0$. Solutions of Eq. (1) can be determined from the appropriate boundary conditions by using the transfer matrix method. The boundary conditions are open in the z direction, and periodic on each slide, that is in the y direction. The former imply plane wave solutions in the z axis, and the latter yield an energy discretization on y . As a consequence, this discretization results in a number of transverse channels equal to the number of points in the transverse mesh direction. Once the solutions are known, the transmission coefficient is computed as a function of the electron energy.

MODEL OF DISORDER

In order to treat lateral disorder, we have considered the occurrence of islands on the interface between two consecutive layers having identical lateral sizes all of them and being consecutive one to each other. In our model, islands have heights (measured from mean position of the heterojunction) that are randomly distributed to mimic random fluctuations of local flux of atoms during growth. It is then feasible to express the rough profile of the interface between two consecutive epilayers defining the following height function

$$h(y) = \eta \sum_n w_n \{ \Theta(y - n\zeta) + \Theta[(n+1)\zeta - y] - 1 \}. \quad (2)$$

Here $h(y)$ represents the deviation from the flat surface at position y , Θ is the Heavyside theta function, ζ is the island width, w_n is a random variable associated to the n th island that controls the fluctuation around the mean value, and η is the largest deviation—in absolute value—assuming that the w_n 's are uniformly distributed between -1 and 1 . Hereafter η will be referred to as degree of *lateral disorder*. The random variables w_n take values from -1 to 1 uniformly, satisfying the following correlator $\langle w_n w_m \rangle = \delta_{nm}/3$, where the brackets indicate average over different realizations of the disorder. In particular, notice that $\langle h(y) \rangle = 0$.

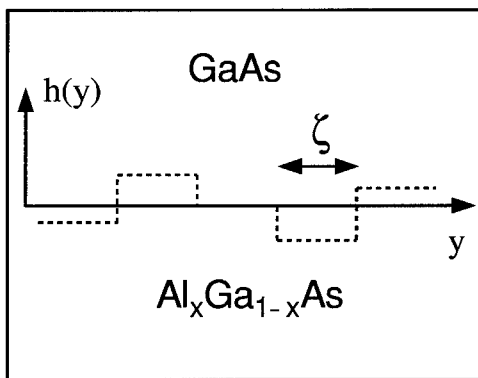


Figure 2. Islands modeling lateral disorder (roughness) at the interface between two epilayers (GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$).

RESULTS

We have performed several numerical calculations in order to study the effect of both lateral and compositional disorder over the transport properties of DBH made of GaAs- $\text{Al}_x\text{Ga}_{1-x}\text{As}$ heterostructures. We start by considering the effect of the interface roughness, characterized by the degree of lateral disorder η given in (2).

Figure 3 shows the transmission coefficient calculated for different values of η . Here $a_y = 10$ nm, $a_z = 0.3$ nm, $\zeta = 20$ nm, $M = 50$, and $N = 38$. The barrier widths are 2.1 nm for both the emitter and the collector, their heights are also the same, 0.3 eV, and the well width is 4.8 nm. Three different values of η were studied, namely $\eta = 0$ (perfect DBH), $\eta = 0.3$ nm (largest fluctuation of the order of one monolayer) and $\eta = 0.6$ nm (largest fluctuation of the order of two monolayers). As a main result, it can be seen in Fig. 3 that increasing the degree of lateral disorder, η , results in a decrease of the transmission probability at the resonant energy. Notice that the resonant peak slightly widens due to the fluctuations of its energy for each realization of the disorder. Besides, an additional effect can be seen, that is, as the degree of lateral disorder η increases the conductance peak shifts to smaller energies. The lowering of the energy of the resonance can be understood assuming that surface roughness makes the effective width of the quantum well larger than its nominal value. This shift would make both the threshold voltage and the negative differential resistance in the current voltage characteristic of DBH to appear at lower bias. But an effective wider well implies a higher current too, so in some statistical sense the current for the disordered DBH will be higher.

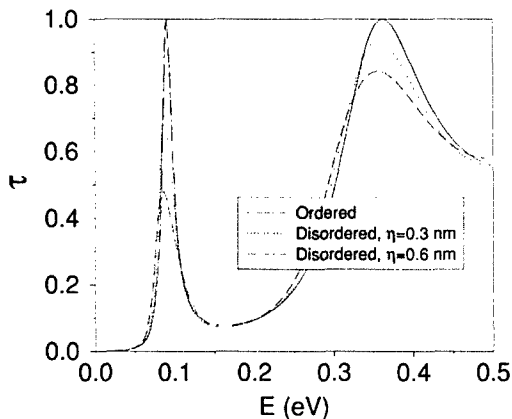


Figure 3. Transmission coefficient through an ordered DBH compared with that of a disordered DBH for two different values of the degree of lateral disorder η . The disordered results comprise 100 realizations of the disorder.

Regarding the effect of the size of the islands, ζ , we have observed that it can be neglected unless this size is of the order of the electron wavelength, that is, for $\zeta \gg \lambda_e$ the transmission coefficient does not depend on ζ . As expected, when $\lambda_e \lesssim \zeta$ the electron starts to see each island and then the transmission coefficient decreases as ζ increases, as shown in Fig. 4. For energies about 0.1 eV this transition takes place at sizes $\zeta \sim 10$ nm [3].

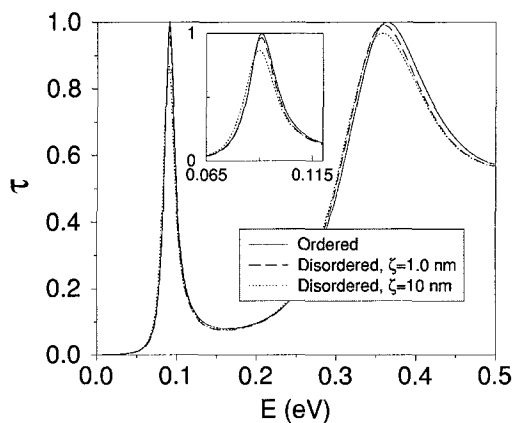


Figure 4. Transmission coefficient through imperfect DBH as a function of the size of the islands for $\zeta \sim \lambda_e$ (dotted line) and $\zeta < \lambda_e$ (dashed line). Curves comprise 50 realizations of the disorder. Inset shows an enlarged view of the main resonance peak.

CONCLUSIONS

In this paper we have presented a method to study electron transmission in unintentionally disordered heterostructures with rough interfaces. We have shown that the main effects of the lateral disorder are to decrease the transmission trough DBH and to lower the resonant energy. As a consequence, our model predicts that the threshold voltage of resonance tunneling diodes becomes smaller in imperfect quantum devices.

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